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Publication date:
2019

Document Version
Publisher's PDF, also known as Version of record

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Molecular Dynamics Supported *In Situ* X-Ray Scattering on Organic Solar Cell Layers

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Motivation

Organic solar cells are presently only used for niche applications due to their semi-transparency, flexibility, low weight, and possibilities of custom designs in terms of colours and shapes, but with their low-cost solution processing and projected energy payback times of only fractions of those of silicon modules, the technology has a great potential to reach commercial viability within few years. However, upscaling the fabrication of organic photovoltaics (OPVs) from laboratory-scale devices to large-scale modules without compromising the device efficiency demands an understanding of the microstructure formation during post-deposition drying of the active layer. By combining the strengths of molecular dynamics (MD) modelling and *in situ* X-ray scattering, we aim to identify the processing parameters that are key to overcome this lab-to-fab challenge and move towards cheap, large-scale, and non-toxic solar cells with record efficiencies.

Simulating post-deposition drying

The efficiency of solution processed OPVs is crucially dependent on the 3D mesoscale thin-film morphology, which in turn is greatly influenced by solvent properties and evaporation rate. In order to reliably simulate active layer morphologies from MD simulations, we have scripted a range of evaporation schemes incorporating e.g. potential walls mimicking substrate– and air interfaces as well as including a suspended solvent vapour above the film from which solvent molecules are continuously removed.[1]

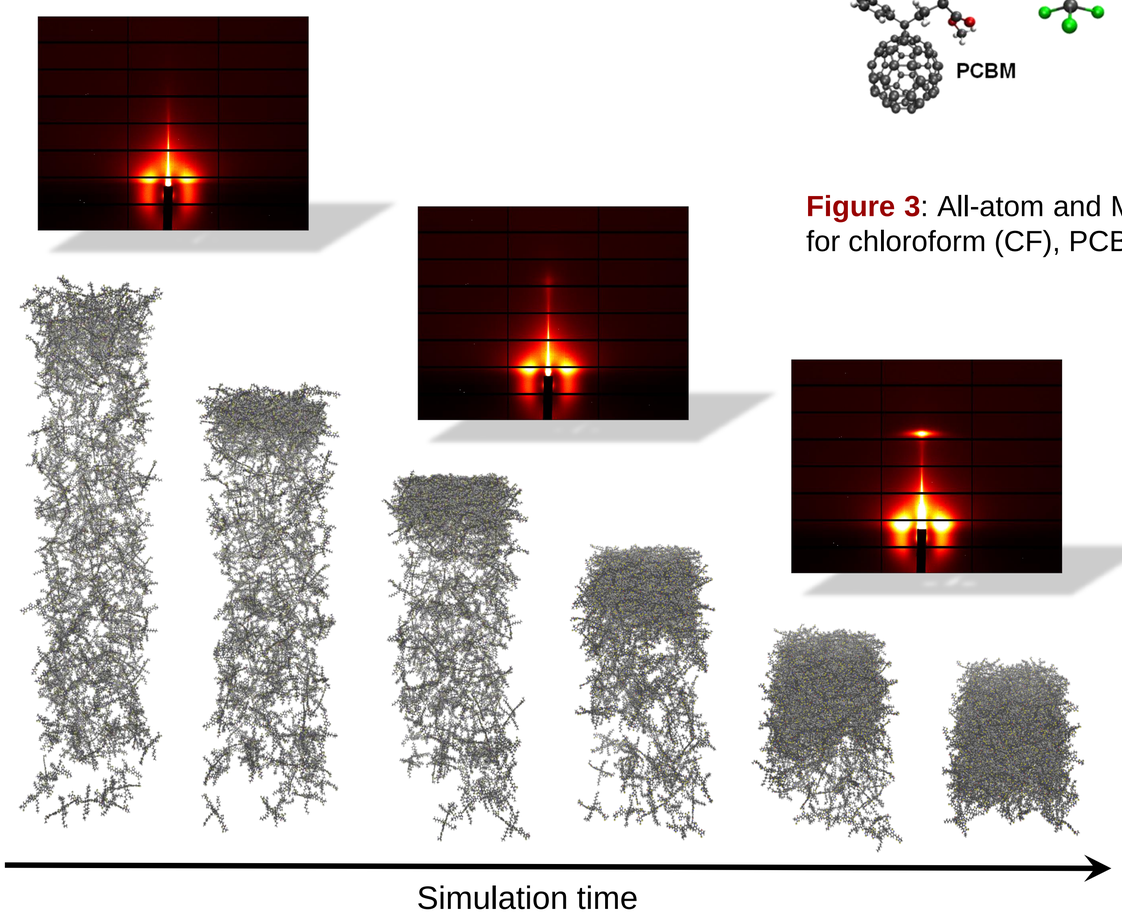


Figure 1: Solvent evaporation simulation and examples of corresponding grazing incidence small-angle X-ray scattering (GISAXS) signals recorded at cSAXS, SLS.

Approaching experimental time-scales

Using the MARTINI force field[2] to coarse-grain our systems, the time- and length-scales relevant for morphology evolution are within reach of MD simulations:[3,4]

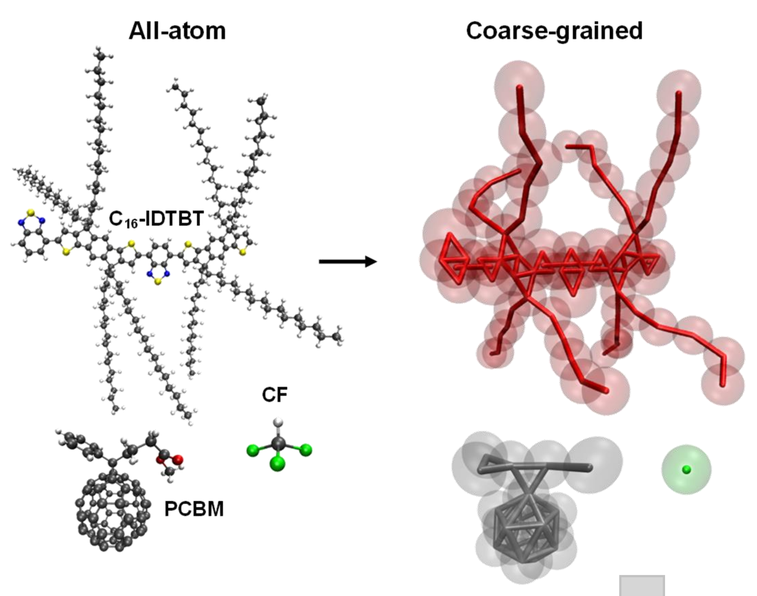
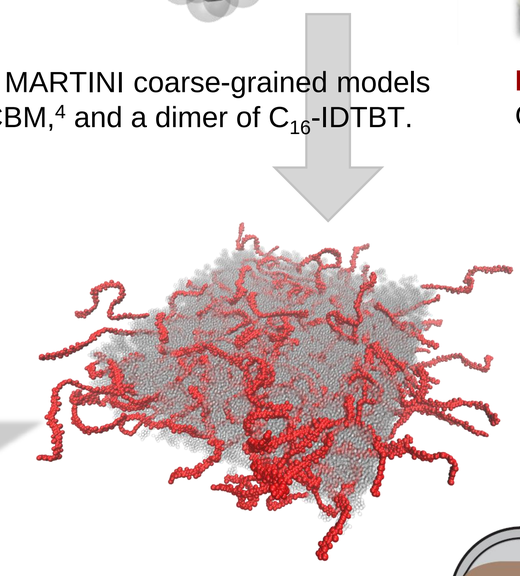
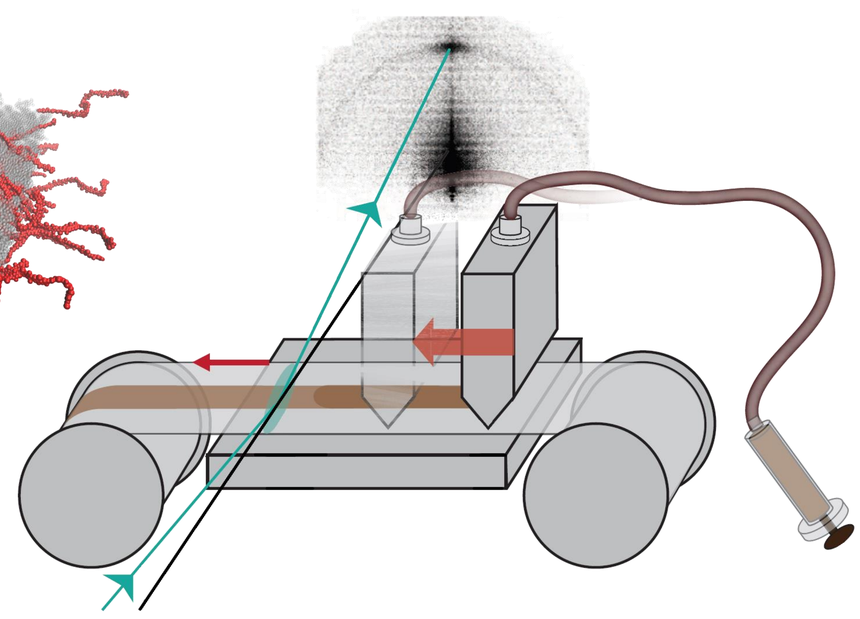


Figure 3: All-atom and MARTINI coarse-grained models for chloroform (CF), PCBM,[4] and a dimer of C_{16}-IDTBT.





Overcoming the lab-to-fab challenge

The knowledge gained from these studies can be used to pin-point the optimal processing conditions for large-scale fabrication of organic solar cells.

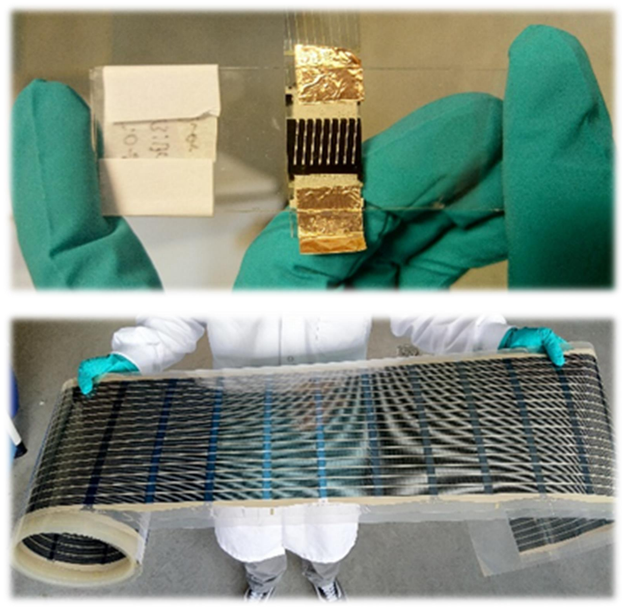


Figure 4: Scalably deposited, flexible OPVs (A. S. Gertsen *et al.,* in peer review, Energy Environ. Sci.).

Figure 2: Schematic of the roll-to-roll slot-die coating setup used for *in situ* GISAXS experiments at the cSAXS beamline, SLS (adapted from Ref. 5).

Acknowledgements

We acknowledge the Paul Scherrer Institute, Villigen, Switzerland for provision of synchrotron radiation beamtime at the cSAXS beamline at SLS, DanScatt for covering travel expenses, and financial support from the H2020 European Research Council through the SEEWHI Consolidator grant, ERC-2015-CoG-681881. ASG thanks the team responsible for the Niflheim supercomputer at DTU where all calculations were performed.

Methodology

We have used the GROMACS 2016.3 package for all MD simulations. The OPLS-AA force field[6] formed the basis for the all atom simulations with our own parameterizations of e.g. most angles and in particular the inter-monomer torsional potentials and sidechain couplings – these were based on quantum chemical DFT calculations. The coarse-grained simulations were based on the MARTINI force field[2] and in part Ref. 4.

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